SHORT ABSTRACT

The thesis entitled **"*Coordination Chemistry and Recognition of Some Metal Ions Using N- or N, O-Donor Ligands*"** has been divided into five chapters based on the results of experimental works performed during the complete course of the PhD research period. **Chapter 1** is the introduction, which describes self-assembly of the coordination complexes by supramolecular interactions based on selected recent literature reports. Some highlights on fluorescence sensors containing different fluorophore moieties for the detection of various metal ions have been described. **Chapter 2** describes molecular structures of nine metal complexes synthesized using a monodentate *N*-substituted imidazole ligand, 1-(4-acetylphenyl)imidazole (**L**) and coligands. Weak interactions present in three pairs of isomorphous and isostructural mononuclear complexes, a mononuclear complex, a 1D coordination polymer and a 2D-coordination polymer have been described. In **Chapter 3**, a trisubstituted imidazole, 2,4-bis(2-pyridyl)-5-(4-pyridyl)imidazole (**L1H**) has been employed which acts as a fluorophore and selectively detect Zn^{2+} ion by a characteristic fluorescence response. The Zn^{2+} ion can be detected within a calculated limit of 6.5×10^{-7} M. A complex of composition $[Zn_2(\mathbf{L1})Cl_3(H_2O)]$ was isolated as a crystalline solid by reacting **L1H** with $ZnCl_2$ which was structurally characterized. In this complex, **L1H** got deprotonated and bound to Zn^{2+} ion in pentadentate fashion as $\mathbf{L1}^-$ ion, by using all the five donor atoms. In **Chapter 4**, two new hydrazones *viz.*, 2-(2-(2,3-dihydroxy)benzylidenehydra-zinyl)benzothiazole (**L2H**) and 2-((2-(2-hydroxy)(4-*N*,*N*-diethylamino))benzylidenehy-drazinyl)benzothiazole (**L3H**), were synthesized which are weakly emissive in nature due to PET process and gave "*turn-on*" responses with $AlCl_3$. The DFT/TDDFT calculations performed on **L2H**, **L3H** and their Al(III) complexes revealed that HOMO-LUMO energy gap got reduced upon complexation. In **Chapter 5**, a hydrazide 6-(hydroxymethyl)-*N*'-((2-hydroxy-1-naphthyl)methylene)picoli-nohydrazide (**L4H**) was synthesized by condensation of 2-hydroxy-1-napthaldehyde and 6-(hydroxymethyl)picoloinohydrazide. This probe acts as "*turn on*" fluorescent sensor for multi detection of Al^{3+}, Zn^{2+} and Cd^{2+} ions at distinct emission maxima. The resultant Al(III) complex gave "*turn–off"* response towards F^- ion. Similar quenching responses were also exhibited in case of Zn^{2+} and Cd^{2+} complexes upon addition of $H_2PO_4^-$ ion. The DFT/TDDFT calculations performed on **L4H**, $[Al(\mathbf{L4})_2]^+$, $[Zn(\mathbf{L4})Cl(H_2O)_2]$ and $[Cd(\mathbf{L4})Cl(H_2O)_2]$ are supported by the experimentally observed results.